

# Kinetics of step bunching during growth: A minimal model

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We study a minimal stochastic model of step bunching during growth on a one-dimensional vicinal surface. The formation of bunches is controlled by the preferential attachment of atoms to descending steps (inverse Ehrlich-Schwoebel effect) and the ratio  $d$  of the attachment rate to the terrace diffusion coefficient. For generic parameters ( $d > 0$ ) the model exhibits a very slow crossover to a nontrivial asymptotic coarsening exponent  $\beta \simeq 0.38$ . In the limit of infinitely fast terrace diffusion ( $d = 0$ ) linear coarsening ( $\beta = 1$ ) is observed instead. The different coarsening behaviors are related to the fact that bunches attain a finite speed in the limit of large size when  $d = 0$ , whereas the speed vanishes with increasing size when  $d > 0$ . For  $d = 0$  an analytic description of the speed and profile of stationary bunches is developed.

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## I. INTRODUCTION

Step bunching is a morphological instability of a vicinal crystal surface in which a regular train of equally spaced steps decomposes into alternating low step density regions (terraces with orientation close to a singular surface) and high step density regions (bunches) [1]. During the evolution the surface self-organizes into a pattern with a characteristic length scale, which coarsens in time. The phenomenon of considerable interest for applications [2] as well as from the fundamental point of view of non-equilibrium statistical mechanics.

Step bunching is generally caused by breaking the symmetry between the ascending (upper) and descending (lower) steps bordering a terrace. This can be due to a variety of mechanisms. In growth or sublimation, the symmetry is broken by different kinetic rates for the attachment or detachment of particles at the upper and the lower step [3], while in electromigration [4] the asymmetry is introduced by the electric field. Other mechanisms responsible for step bunching during growth include impurities [5, 6], diffusion anisotropy [7], and the presence of a second surface species [8]. Quite generally, a growing equidistant step train shows a step bunching instability when adatoms attach to the step more easily from the upper terrace than from the lower terrace (an *inverse Ehrlich-Schwoebel effect*, iES). While iES behavior is difficult to justify microscopically, it may serve as a useful *effective* description of more complex step bunching mechanisms [7].

The coarsening of the bunched surface can be characterized by the power law increase of the average distance between bunches  $\mathcal{L}$  as  $\mathcal{L} \propto t^\beta$ . A few experimental observations of step bunch coarsening during growth have been reported [7, 9, 10, 11], but quantitative results are scarce. Numerical simulations of the equations of step

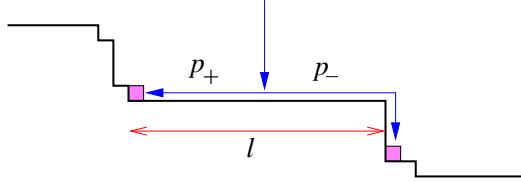


FIG. 1: Illustration of the model. Particles are deposited onto the terraces and attach to the ascending (descending) step with probability  $p_+$  ( $p_-$ ). The attachment probabilities depend on the terrace width  $\ell$  through (1).

motion found  $\beta = 1/2$  independent of the step interaction potential [12]. Recently a unifying continuum treatment of step bunching instabilities was proposed [13, 14, 15] with the aim to identify *universality classes*. Nevertheless, a good understanding of the relationship between microscopic step bunching mechanisms and the resulting asymptotic scaling properties is so far lacking.

In this paper, we study coarsening of step bunches during growth for a simple one-dimensional lattice model. The main idealization compared to conventional one-dimensional models [12] is that repulsive step-step interactions are ignored, and hence the individual steps can coalesce to form composite steps. This eliminates the internal structure of the bunch and the associated additional length scale [14], and allows us to simulate large systems over very long times. Related models have been proposed previously [9, 10, 16, 17], but their asymptotic bunching behavior has not been explored.

## II. MODEL

We consider  $S$  steps of unit height located at positions  $x_1, x_2, \dots, x_S$  of a one-dimensional lattice with  $L$  sites and periodic boundary conditions; the slope of the vicinal surface is  $m_0 = S/L$ . The width of the  $i$ -th terrace between steps  $i$  and  $i-1$  is  $\ell_i = x_i - x_{i-1}$ . Due to the ab-

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sence of step-step repulsion two or more steps can be located at the same position; correspondingly some terrace widths may be zero. Particles are uniformly deposited onto the sample. A particle deposited on a terrace of width  $\ell$  moves immediately to one of the bordering steps and is incorporated with the probabilities

$$p_{\pm} = \frac{1}{2} \frac{1 \pm b + d\ell}{1 + d\ell} \quad (1)$$

at the ascending ( $p_+$ ) or descending ( $p_-$ ) step, respectively (Fig. 1). The *balance*  $b$  is a measure for the attachment asymmetry, while the *inverse diffusivity*  $d$  determines how the asymmetry depends on the width of the terrace: For  $d = 0$  the attachment probabilities  $p_{\pm}$  are independent of the terrace width, while for  $d > 0$  the attachment becomes symmetric when  $\ell \gg 1/d$ . Note that in the symmetric case ( $b = 0$ ) the value of  $d$  is irrelevant. For  $d = 0$  and  $b = 1$  the model is exactly solvable, and the terrace widths have a Poisson distribution [17].

The form (1) follows from the solution of the stationary diffusion equation for the adatoms on the terrace [1, 18], which leads to the following expressions for the model parameters in terms of the adatom diffusion coefficient  $D$  and the attachment rates  $k_{\pm}$  [1, 3]

$$b = \frac{k_+ - k_-}{k_+ + k_-} \quad (2)$$

$$d = \frac{1}{D/k_+ + D/k_-} \quad (3)$$

A normal Schwoebel effect ( $k_+ > k_-$ ) corresponds to  $b > 0$ , while an iES effect implies  $b < 0$ . The quantity  $d$  is the inverse of the sum of the kinetic lengths  $D/k_{\pm}$  [1].

As initial condition, the steps are placed at random. We use sample sizes ranging from  $L = 5 \times 10^4$  to  $10^6$ . Time is measured in number of monolayers (ML), and simulations were performed up to  $10^7$  ML. As expected, the model exhibits step bunching when  $b < 0$ . An example of the formation and time evolution of bunches for  $d = 0$  is shown in Fig. 2. Bunches and steps move to the right. Eventually in the stationary regime only a single bunch remains which moves with a constant velocity. In the case  $d > 0$  the coarsening is slower but the space-time plot is qualitatively similar. We observed that the bunch velocity is generally increasing with decreasing  $d$  and increasing  $|b|$  (see Sect. IV for further discussion).

The simplest way to characterize the surface morphology is to measure the surface width  $W$  relative to the mean tilted surface [19]. For  $b \geq 0$  no step bunches form and the surface is roughened only by fluctuations. For  $b > 0$  the model belongs to the Edwards-Wilkinson universality class and  $W \sim t^{1/4}$  [17]. For  $b = 0$  we find numerically that  $W \sim t^{1/3}$ , which is consistent with the idea [20] that the symmetric model belongs to the conserved Kardar-Parisi-Zhang universality class [19]. In the step bunching regime  $b < 0$  the surface width should asymptotically become proportional to the bunch spacing  $\mathcal{L}$ .

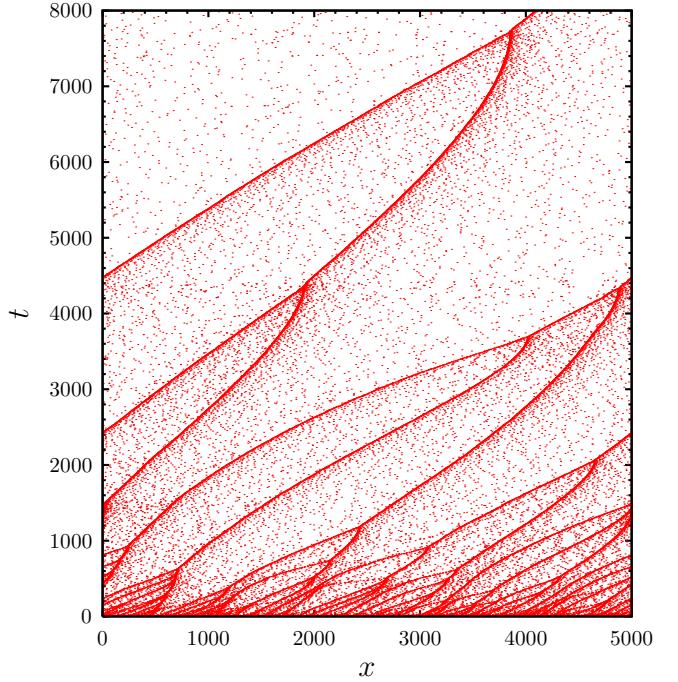


FIG. 2: Spatiotemporal evolution of the step configuration on a vicinal surface of mean slope  $m_0 = 0.2$ . Time is increasing from bottom to top. The positions of the steps are shown as dots. The sample size in the horizontal direction is  $L = 5000$ . Parameters are  $d = 0$  and  $b = -0.6$ .

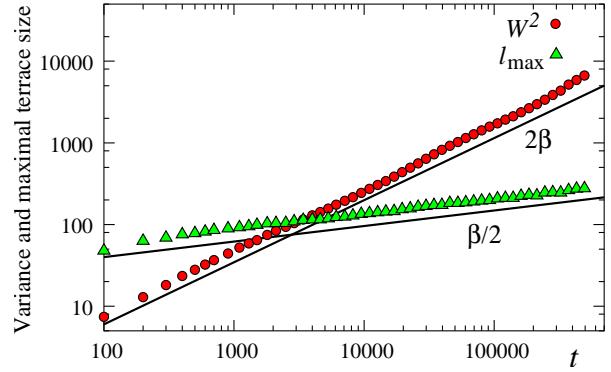


FIG. 3: Squared surface width  $W^2$  and maximal terrace size  $l_{\max}$  as a function of time for a system of size  $L = 2 \times 10^5$ , slope 0.1, and parameters  $b = -1$ ,  $d = 0.1$ . The bold lines have slope  $2\beta = 0.76$  and  $\beta/2 = 0.19$ , respectively.

Indeed we find that  $W$  increases faster than  $t^{1/3}$  when  $b < 0$  (see Fig. 3), but the large background contribution to  $W$  which arises from random fluctuations makes this quantity less suited for a precise determination of the coarsening behavior. We therefore developed an alternative coarsening measure which we describe next.

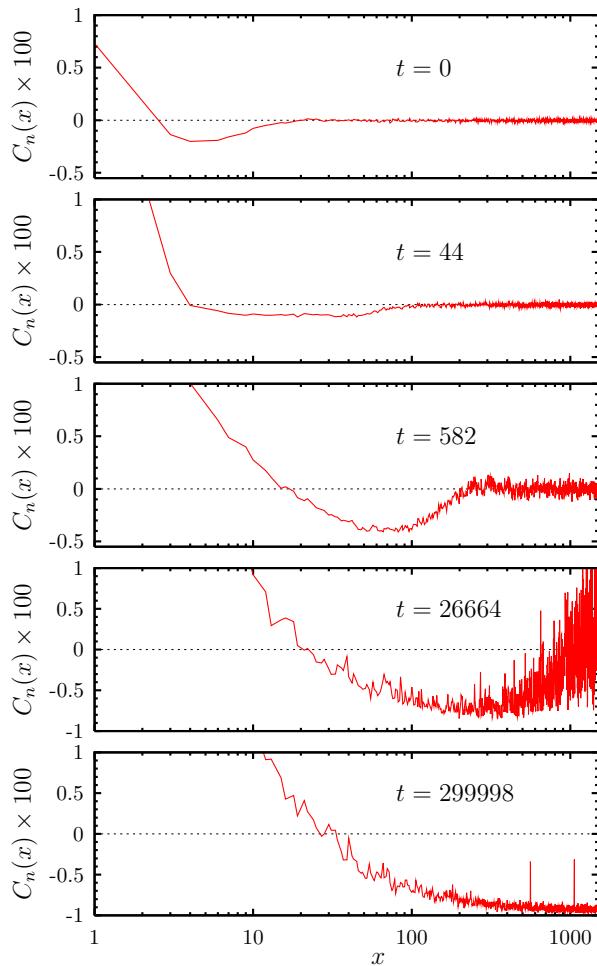


FIG. 4: Density-density correlation function for a system of size  $L = 3000$ , parameters  $b = -0.3$  and  $d = 0.01$ , and mean slope of the vicinal surface equal to 0.1. The data are averaged over 500 independent runs.

### III. COARSENING BEHAVIOR

There are different possible ways to quantitatively analyze the coarsening process. In analogy with phase ordering kinetics [21], we calculated the density-density correlation function

$$C_n(x, t) = \frac{1}{L} \sum_y \langle n(y, t) n(y + x, t) \rangle, \quad (4)$$

the step density being defined as

$$n(x, t) = \sum_{i=1}^S \delta(x - x_i(t)), \quad (5)$$

where  $\delta(x) = 1$  for  $x = 0$  and zero otherwise.

The typical time evolution of the correlation function is plotted in Fig. 4. We observed a minimum in the density-density correlation function, which shifts to larger values

during growth and ultimately saturates at half the system size. We did not observe any significant secondary maximum in  $C_n(x, t)$ , indicating that there is no systematic periodicity in the bunch configurations. The position of the minimum is a good indicator of the typical bunch distance. On the other hand, it is hardly measurable with sufficient precision. Even after averaging over 500 independent runs the results are not satisfactory. Therefore, we turned to other quantities to effectively capture the dynamics of bunching.

We may operationally define a composite step of size  $k$  as an object in which there are at least  $k$  steps at the same position. For  $k = 1$  we are dealing with the steps themselves, while  $k > 1$  corresponds to composite steps in the strict sense. Denote by  $S_k$  the number of such composite steps and  $x_{k,i}, i = 1, 2, \dots, S_k$  their positions. If we identified the step bunches with composite steps and measured the average bunch distance as  $L/S_k$ , we would make a systematic error, because often two such “bunches” come very close one to the other, effectively making up a single larger bunch. We need to eliminate these short distances. To this end we define the quantity

$$\Delta_k = \frac{1}{L} \sum_{i=1}^{S_k} \langle (x_{k,i} - x_{k,i-1})^2 \rangle, \quad (6)$$

in which larger distances dominate over shorter ones. Therefore, the quantity  $\Delta_1$  measures the effective distance between steps in regions of low density of steps, i.e. around the middle between the bunches. On the other hand,  $\Delta_k$  for  $k > 1$  measures the effective distance between bunches, irrespective of the elementary steps dispersed between bunches.

We compared the time evolution of  $\Delta_k$  for various values of  $k$ . As expected, the behavior differs qualitatively for  $k = 1$  and for  $k > 1$ . The quantity  $\Delta_1$  grows with time and eventually saturates at a value which is significantly lower than the system size. The saturated value increases with increasing  $|b|$  and approaches the system size for  $b \rightarrow -1$ .

On the other hand, the quantities  $\Delta_k$  for  $k > 1$  exhibit first a transient period with a fast decrease and then grow until they reach a value very close to the system size. (In principle the quantity is always lower than the system size, but we observed that this difference becomes negligible when we increase the system size. This fact can be easily understood from the form of the stationary bunch profile, as will be shown below in Sect.IV B). The behavior depends on  $k$  only in the initial transient period, which is longer for larger  $k$ . However, the universal long time behavior, which is the subject of this work, is found to be independent of  $k > 1$ . Therefore, we will concentrate on the quantity  $\Delta_2$  in the following.

We investigated the time evolution of the distance between bunches in different regimes depending on the parameters  $b$  and  $d$ . Typical results are shown in Fig. 5 for  $b = -0.9$  and several values of the diffusion parameter  $d$  (the results for other values of  $b < 0$  are similar).

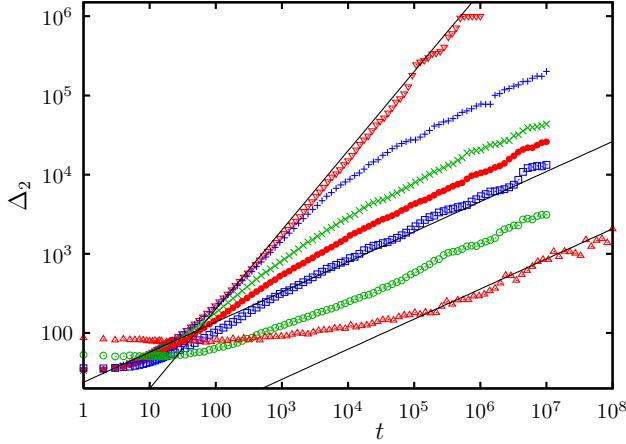


FIG. 5: Time evolution of the distance between bunches measured by  $\Delta_2$  for  $b = -0.9$ , and varying diffusion parameter  $d = 0, 0.0001, 0.001, 0.003, 0.01, 0.1$ , and  $1$  (from top to bottom at time  $10^5$ ). System sizes are  $10^6, 10^6, 5 \times 10^5, 5 \times 10^5, 10^5, 10^5$ , and  $5 \times 10^4$ , respectively. The lines are powers  $\propto t^1$  and  $t^{0.38}$ . The mean slope of the vicinal surface is  $0.2$ .

For  $d = 0$ , linear behavior  $\Delta_2 \propto t$  is reached after some transient, i.e.  $\beta \approx 1$ . On the other hand, the situation for nonzero  $d$  is more complex. After the initial transient, there is an intermediate behavior with approximately power-law character, but the exponent strongly depends on the value of  $d$ , while the dependence on  $b$  was very weak.

Eventually, after some crossover time  $\simeq t_c$  a stationary power-law regime is reached, which in our data extends over several orders of magnitude in time. The effective exponent  $\beta$  is only weakly varying with the nonzero  $d$  and assumes the asymptotic value  $\beta \simeq 0.38$ . We conjecture that this regime is universal and the remaining variations in the value of the exponent are solely due to finite size effects.

In order to confirm that the asymptotic behavior is universal, one can rescale the raw data for different nonzero  $d$ , plotting them as functions of  $t/t_c$  in the form

$$\Delta_2(t; b, d) = \Delta_{2z} + (t/t_c)^{0.38} \Delta_{2c} F(t/t_c). \quad (7)$$

The results for three values of  $d$  and three values of  $b$  are shown in Fig. 6. Neglecting the initial transient, we see that the scaling function  $F(x)$  approaches unity for  $x \gg 1$ , marking the asymptotic universal regime, and behaves close to a power-law  $F(x) \sim x^\tau$  for  $x \ll 1$ , which characterizes the intermediate regime; the exponent  $\tau$  depends on  $d$  but is independent of  $b$ . The initial offset  $\Delta_{2z}$  was introduced for convenience.

The crossover time  $t_c$  between the intermediate and asymptotic regimes turned out to be rather large ( $t_c \simeq 10^4$  for  $d = 0.001$  and  $b = -0.9$ ) and it increases rapidly with decreasing  $|b|$ , as can be seen in the inset of Fig. 6, where behavior consistent with a power law  $t_c \sim (-b)^{-4}$

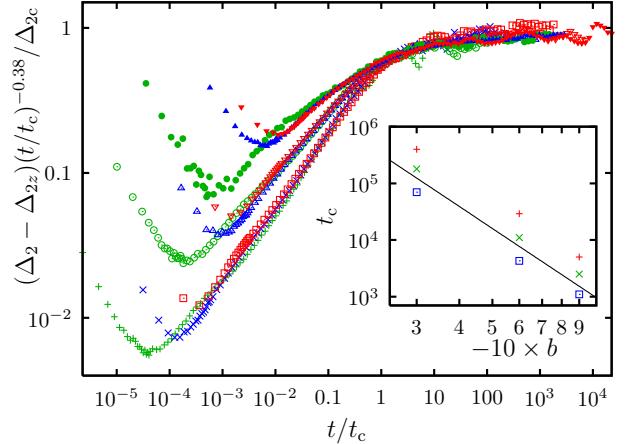


FIG. 6: Scaled time evolution of the effective distance between bunches measured by  $\Delta_2$  for three values of the balance and three values of the inverse diffusivity. Groups of curves correspond to diffusion parameters  $d = 0.01, 0.001, 0.0001$  from top to bottom. Each group consists of data for  $b = -0.9$  ( $\square$ ,  $\nabla$ ,  $\blacktriangledown$ ),  $-0.6$  ( $\times$ ,  $\triangle$ ,  $\blacktriangle$ ), and  $-0.3$  ( $+$ ,  $\odot$ ,  $\bullet$ ). The slope of the vicinal surface and the sample sizes are the same as in Fig. 5. The inset shows the values of the crossover time  $t_c$  used in the main plot. The values of  $d$  are  $10^{-4}$  ( $+$ ),  $10^{-3}$  ( $\times$ ), and  $0.01$  ( $\square$ ). The line is a power law  $\propto (-b)^{-4}$ .

is apparent. The dependence on  $d$  turns out to be non-monotonic: The crossover time decreases up to about  $d = 0.01$  and then increases again. This shows that different crossover mechanisms are acting for small and large  $d$ , respectively.

Indeed, for very small  $d$  the dependence of the attachment asymmetry on the terrace size is felt only once the terraces become sufficiently large, and the system behaves initially as if  $d = 0$  and  $\beta = 1$ ; correspondingly the coarsening exponent approaches its asymptotic value from above in this case. Conversely, for large  $d$  the asymmetry in the attachment probabilities (1) is always very small; consequently it takes a long time for the bunches to form, and the asymptotic coarsening exponent is approached from below.

The asymptotically linear behavior of the bunch size for  $d = 0$ ,  $\beta \approx 1$ , is well confirmed by measurements of the surface width  $W$ , and the data for  $d = 0.1$  shown in Fig. 3 are consistent with the estimate  $\beta \approx 0.38$  obtained from  $\Delta_2$ . In addition, Fig. 3 displays the evolution of the maximal terrace width  $\ell_{\max}$  in the system. This length scale is seen to scale with a distinct exponent which is approximately given by  $\beta/2 \approx 0.19$ . We will return to the behavior of  $\ell_{\max}$  below in Sect. IV B.

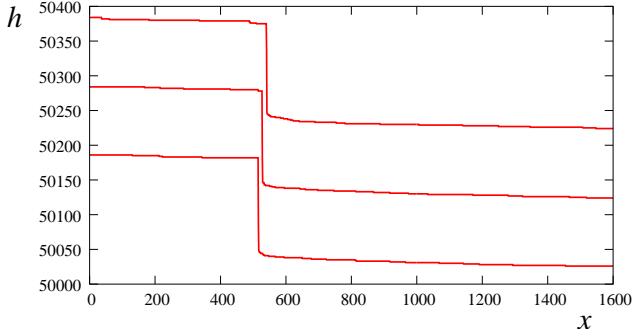


FIG. 7: Height profiles of a stationary bunch for  $d = 0$ ,  $b = -0.1$ . The figure shows a surface with  $S = 160$ ,  $L = 1600$  after deposition of 50000, 50100 and 50200 ML, respectively.

#### IV. STATIONARY BUNCHES

The final state of the system for any  $b < 0$  is found to be a single bunch propagating at constant velocity (Fig.7). The analysis of these stationary configurations provides important clues to the different coarsening behaviors observed for  $d = 0$  and  $d > 0$ , respectively.

##### A. Bunch speed

Figure 8 shows numerical results for the stationary bunch speed  $v$ . For  $d = 0$ ,  $v$  approaches a finite limiting value  $v_\infty$  with increasing system size; this is also evident from the space-time plot in Fig.2. The bunch speed is easily determined for the limiting case  $d = 0$ ,  $b = -1$ . In this limit single steps cannot detach from the bunches, and the formation of composite steps is irreversible. The motion of a bunch is solely due to the atoms deposited onto the trailing terrace behind the bunch, which has length  $L$  in the stationary state. To move the bunch containing all  $S$  steps laterally by one lattice spacing,  $S$  atoms have to be deposited on this terrace; the bunch speed is therefore  $v_\infty = L/S = 1/m_0$ . The limiting bunch speed decreases with decreasing  $|b|$  and vanishes as  $v_\infty \sim b^2$  for  $b \rightarrow 0$  (see inset of Fig.8). An analytic explanation of this behavior will be given below in Sect.IV C.

For  $d > 0$  the bunch speed decreases indefinitely with increasing  $L$ . The simulation results shown in Fig.8 are consistent with a behavior

$$v(L) \sim L^{-\nu} \quad (8)$$

with  $\nu \approx 1$ , but owing to the significant curvature of the data, the asymptotic value of  $\nu$  cannot be accurately determined.

Following a simple scaling argument due to Chernov [22], we can try to relate the exponent  $\nu$  in (8) to the coarsening exponent  $\beta$ . At a time when the typical bunch spacing is  $\mathcal{L}$ , the bunch speeds are of order  $\mathcal{L}^{-\nu}$ . Assuming that there is only a single scale in the problem, the

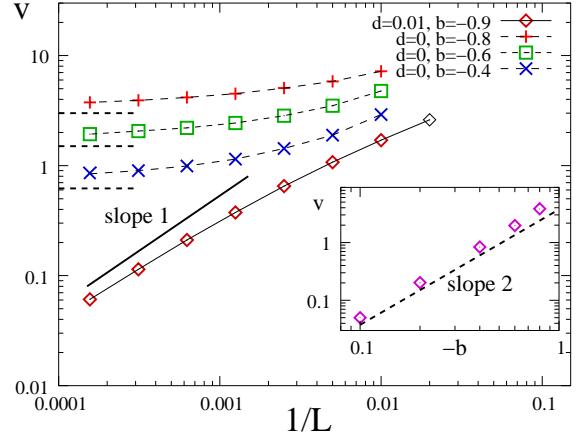


FIG. 8: Propagation speed  $v$  of stationary bunches. The main plot shows the dependence of  $v$  on the system size  $L$ , contrasting the behavior for  $d = 0$  and  $d > 0$ . The inset shows the bunch speed for  $d = 0$ , extrapolated to  $L = \infty$ , as a function of  $|b|$ ; the extrapolation is based on data up to  $L = 1600$  and assumes a leading correction of order  $1/L$ . All data were obtained by time averages in the stationary regime. The surface slope was 0.1 for  $d = 0$  and 0.2 for  $d = 0.01$ . The full bold line illustrates the behavior  $v \sim 1/L$ . The dashed bold lines are the *upper* bounds on  $v$  derived in Sect.IV C. The bounds in the main figure were derived from the algebraic equation (21), while the bound in the inset is the inequality (16) which becomes exact for  $|b| \rightarrow 0$ .

velocity difference  $\Delta v$  between two bunches is of the same order. The time  $t^*$  until the coalescence of two bunches can then be estimated as  $t^* \sim \mathcal{L}/\Delta v \sim \mathcal{L}^{1+\nu}$ , and reversing this relationship one obtains the expression

$$\beta = \frac{1}{1 + \nu} \quad (9)$$

for the coarsening exponent. For  $d = 0$  we have seen that the bunch speed remains finite for  $L \rightarrow \infty$ , hence  $\nu = 0$  and  $\beta = 1$  in agreement with the coarsening simulations.

For  $d > 0$  the value  $\nu \approx 1$  implies  $\beta \approx 1/2$ , which is larger than our numerical estimate  $\beta \approx 0.38$ . Although the data for  $v(L)$  in Fig.8 are probably not asymptotic, it seems unlikely that they will ever reach the large slope  $\nu \approx 1.6$  required to reproduce our value for  $\beta$ . In fact, our simulations show clearly that, besides the coalescence of bunches, the exchange of steps between bunches of different size plays an important role in the coarsening process. In addition, the existence of the distinct length scale  $\ell_{\max}$  (see Fig.3) invalidates the assumption that the bunch spacing is the only length scale in the problem. Thus, while Chernov's relation (9) helps to connect the different coarsening behaviors for  $d = 0$  and  $d > 0$  with the difference in the size dependence of the bunch speed on a qualitative level, it is not quantitatively satisfied for our model.

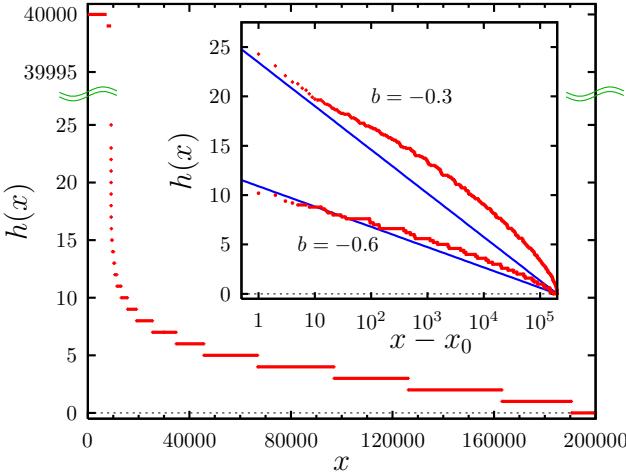


FIG. 9: Stationary bunch profile at time  $1 \times 10^7$  for sample size  $L = 2 \times 10^5$  with slope 0.2 for  $d = 0$  and balance  $b = -0.3$ . Inset shows log-linear plot of profile relative to the center of bunch  $x_0$ , averaged over 11 (for  $b = -0.3$ ) and 5 (for  $b = -0.6$ ) independent runs. The lines are predictions from the formulae (10) and (21).

### B. Height profile

We measured the height profile between bunches in the stationary regime. We show in Fig. 9 the results for  $d = 0$  and two values  $b = -0.3$  and  $b = -0.6$ . Qualitatively we observe that for larger values of  $-b$  the bunch becomes steeper in its very center, while the rest of the bunch, farther from the center, is more gradual. Since there is no repulsion between steps they tend to accumulate in the center of bunch (position denoted  $x_0$ ) and to the right of it, while the region on the left-hand side is much more flat. This means that the bunch shape is strongly asymmetric. Due to the discreteness of the lattice it is very difficult to infer precisely the singular behavior near the center of bunch, but the averaged data in the inset show that the profile far from the center can be described by a logarithmic behavior of the form

$$h(x_0) - h(x) \approx A \ln(x - x_0). \quad (10)$$

The logarithmic singularity observed in the bunch shape is very weak and in all cases investigated most of the mass of the bunch is concentrated on two sites in its center. Indeed, setting  $x - x_0 = L$  in (10) it is seen that the number  $S_t$  of terrace steps which are not contained in the center of the bunch grows only logarithmically with  $L$ . This is the ultimate reason why the effective quantity  $\Delta_2$  measures quite well the distance between bunches.

The logarithmic height profile implies that the surface slope  $m(x) = \partial h / \partial x$  decays as  $m(x) \approx -A/x$  far away from the bunch. The size  $\ell_{\max}$  of the largest terrace in the system, which is found at a distance of order  $L$  from the bunch, is then of order  $\ell_{\max} \sim -m(L) \sim L$ . This is consistent with measurements of  $\ell_{\max}$  for stationary

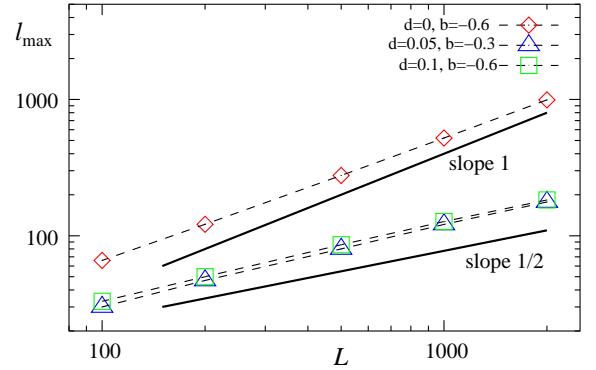


FIG. 10: Maximal terrace size  $\ell_{\max}$  for stationary bunches as a function of system size  $L$ . The mean slope is  $m_0 = 0.2$ . The data were obtained as time averages over single runs.

bunches with  $d = 0$  (Fig.10). On the other hand, for  $d > 0$  the largest terrace is much smaller, and scales approximately as  $\ell_{\max} \sim L^{1/2}$ . This matches the time-dependent behavior of  $\ell_{\max}$  shown in Fig.3.

### C. Analytic description of stationary bunches

In this section we provide an analytic derivation of several of the numerically observed properties of stationary bunches for the case  $d = 0$  [25]. A convenient starting point is the continuum evolution equation

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x} \left[ -\frac{|b|}{2m} + \frac{1}{6m^3} \frac{\partial m}{\partial x} \right] = 1, \quad (11)$$

which has been obtained for the deterministic version of the present model through an essentially rigorous coarse graining procedure [18, 20]. Here  $m = \partial h / \partial x$  is the surface slope, the time scale is chosen such that the deposition flux equals unity, and  $b$  is assumed negative. A continuum description of the type (11) is expected to be valid far ahead of the bunch, where the step spacing is large compared to the atomic scale and lattice effects are negligible.

We are looking for solutions of (11) which describe a bunch of height  $S$  (in units of the vertical lattice spacing) in a system of length  $L$ , moving laterally at speed  $v$ . This implies the ansatz

$$h(x, t) = f(x - vt) + \Omega t, \quad (12)$$

where the last term accounts for the fact that also the regions between bunches grow vertically due to the terrace steps that move across these regions [23] (see Fig.7). The constant unit flux on the right hand side of (11) implies the sum rule [24]

$$\Omega + \frac{S}{L} v = 1 \quad (13)$$

connecting the vertical and lateral growth rates. Inserting (12) into (11) one obtains the ordinary differential

equation

$$-vg + \frac{d}{d\xi} \left[ -\frac{|b|}{2g} + \frac{1}{6g^3} \frac{dg}{d\xi} \right] = 1 - \Omega \quad (14)$$

where  $\xi = x - vt$  and  $g = df/d\xi$  is the surface slope in the comoving frame. The first term on the left hand side of (14) can be neglected relative to the right hand side when  $g \ll m_0$ , which is true far ahead of the bunch. Then it is readily verified that the equation admits a solution of the form  $g(\xi) = -A/\xi$ , consistent with the height profile (10). The coefficient  $A$  satisfies the quadratic equation

$$(1 - \Omega)A^2 - A|b|/2 + 1/6 = 0. \quad (15)$$

Using (13), one finds that (15) has real solutions only when the bunch speed satisfies the inequality

$$v \leq \frac{3}{8} \frac{b^2}{m_0}. \quad (16)$$

Whereas the proportionality  $v \sim b^2$  suggested by this relation is well confirmed by the data in the inset of Fig.8, the bound on the numerical coefficient seems to be weakly violated by the data. However, since the convergence of  $v$  with increasing  $L$  is quite slow, we believe that our simulations can still be regarded to be consistent with (16). Assuming that (16) is satisfied essentially as an equality, we find that the coefficient  $A$  is given by

$$A = \frac{2}{3|b|}. \quad (17)$$

The relations (16) and (17) can be improved by analyzing the discrete evolution equations for the mean step positions  $X_i = \langle x_i \rangle$ . For  $d = 0$  they take the simple linear form [3, 20]

$$\frac{dX_i}{dt} = \frac{1}{2}(1+b)(X_{i+1} - X_i) + \frac{1}{2}(1-b)(X_i - X_{i-1}). \quad (18)$$

The moving bunch is described by a solution of the form

$$X_i(t) = \phi(i + \Omega t) + vt, \quad (19)$$

where  $\Omega$  and  $v$  have the same meaning as in (12). Inserting (19) into (18) one obtains the difference-differential equation

$$v + \Omega \frac{d\phi}{d\zeta} = -b\phi(\zeta) + \frac{1}{2}(1+b)\phi(\zeta+1) - \frac{1}{2}(1-b)\phi(\zeta-1) \quad (20)$$

for the function  $\phi(\zeta)$ , where  $\zeta = i + \Omega t$ . The expected logarithmic height profile (10) corresponds to an exponential increase of  $\phi$  as  $\phi(\zeta) \sim e^{\zeta/A}$ . For large  $\zeta$  the constant  $v$  on the left hand side of (20) can be neglected. Inserting the exponential ansatz into (20) yields the algebraic equation

$$\Omega = A \{ \sinh(1/A) + |b| [1 - \cosh(1/A)] \}, \quad (21)$$

which reduces to (15) for small  $|b|$  and large  $A$ . For general values of  $|b|$ , (21) has real solutions only when the bunch speed  $v$  is smaller than an upper bound  $v_{\max}(b)$ , which reduces to (16) for small  $|b|$ . In Figs.8 and 9 we compare the predictions for  $v_{\max}$  and  $A$  derived from (21) with our numerical results. For  $A$  we use the value obtained from (21) under the assumption that  $v = v_{\max}$ , which leads to a rather satisfactory agreement.

## V. CONCLUSIONS

In this paper we have developed and studied a one-dimensional stochastic growth model which contains some essential features of the formation and coarsening of step bunches. Despite its simplicity, the model displays two distinct scaling regimes. In the limit of fast terrace diffusion ( $d = 0$ ) we have numerically established a linear coarsening law ( $\beta = 1$ ) and related this behavior to the fact that the propagation speed of bunches tends to a finite value with increasing bunch size.

When the diffusivity is finite ( $d > 0$ ) the attachment asymmetry decreases with increasing terrace size and the coarsening is slowed down. After having accounted for a complicated crossover behavior, we identified the asymptotic value of the coarsening exponent, which we estimate to be  $\beta \simeq 0.38$ . This exponent is different from exponents found in previous studies of step bunching, and it does not seem to follow from any simple scaling argument. It is robust, in the sense of being independent of the precise values of the model parameters, provided  $b < 0$  and  $d > 0$ .

Similar to earlier studies of kinetic roughening [26], our work shows that finding the true asymptotic exponent may require a considerable amount of computer power due to a long intermediate regime with non-universal, apparent power-law behavior. The situation becomes even more difficult when we try to observe the crossover from  $\beta = 1$  to  $\beta \simeq 0.38$ , which should occur for sufficiently small but non-zero  $d$  and large enough system size  $L$ . Currently this is beyond our capacity.

Due to the absence of step-step interactions, our model cannot provide an accurate description of the structure and dynamics of real step bunches. Nevertheless our study clarifies some conceptual issues that arise also for more realistic models. For example, although the internal width of the bunches has been eliminated by allowing steps to coalesce, the model still displays (for  $d > 0$ ) a second length scale, the maximum terrace size  $\ell_{\max}$ , which grows with an exponent that is distinct from the coarsening exponent. This invalidates simple scaling arguments [13, 14, 22] which assume the bunch spacing to be the only scale in the problem, and which would imply a "superuniversal" coarsening exponent  $\beta = 1/2$  [27].

A second important advance of our work is the demonstration that continuum evolution equations can be used to quantitatively describe the profile and speed of moving step bunches. So far the use of continuum approaches

in step bunching has been limited to scaling arguments [13] and to the study of stationary bunch configurations [15, 27].

To conclude, we speculate that the relationship between growing stepped surfaces and interacting particle systems (specifically, zero range processes [28]) that was pointed out some time ago [20] may be usefully exploited to gain further insight into the coarsening behavior of step bunches. In the language of interacting particle systems, step bunching is an example of a *condensation transition*, where a macroscopic fraction of the particles (i.e., the single height steps in our model) condenses into a few or a single site. The dynamics of such condensation transitions is of great current interest [28, 29], and closely

related concepts appear e.g. in granular physics [30, 31] and traffic research [20, 32].

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